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# Thermodynamic Cycle and CFD Analyses for Hydrogen Fueled Air-Breathing Pulse Detonation Engines

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# THERMODYNAMIC CYCLE AND CFD ANALYSES FOR HYDROGEN FUELED AIR-BREATHING PULSE DETONATION ENGINES

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## Abstract

This paper presents the results of a thermodynamic cycle analysis of a pulse detonation engine (PDE) using a hydrogen-air mixture at static conditions. The cycle performance results, namely the specific thrust, fuel consumption and impulse are compared to a single cycle CFD analysis for a detonation tube which considers finite rate chemistry. The differences in the impulse values were indicative of the additional performance potential attainable in a PDE.

## Introduction

Previous studies have demonstrated the impact of dissociation in propulsion engines.<sup>1</sup> A significant reduction in the sensible heat release available for conversion into thrust occurs due to high temperature dissociation of the burning gases. A subsequent analysis<sup>2</sup> was performed in which the specific thrust, fuel consumption and impulse were compared for a ramjet, a gas turbine and a PDE. In that study, it was found that a PDE has comparable performance with a ramjet over a wide Mach number range. In comparison with a turbojet the PDE was found to be competitive only when the turbojet was operated with a low mechanical compression ratio. More recently, a single cycle CFD analysis was performed for a detonation tube,<sup>3</sup> which included finite rate chemistry modeling.

It was found that some recombination took place in the burning gases behind the detonation front.<sup>3</sup> The recombination served to decrease the amount of

sensible heat loss that occurred during the detonation process due to dissociation

This paper examines the effect of the real gas chemistry, using a combination of the single cycle CFD and the thermodynamic cycle calculations for hydrogen/air mixtures. The results are used to establish the actual performance of a PDE versus the maximum performance potential.

## Analyses

### Thermodynamic Cycle

The thermo cycle analysis used was that developed by Heiser and Pratt<sup>4</sup> and modified in reference 2 for variable gamma and specific heat ratio and for variable reference conditions. The analysis is a classical closed cycle analysis that is independent of time. The significant parameters of the analysis are the thermal efficiency and the sensible heat release, which can be converted into thrust. Those values can be used to calculate all of the usual performance parameters, such as specific thrust, fuel consumption and impulse. In this manner, the maximum performance capability for a pulse detonation engine can be established.

In order to perform the cycle analysis, it is necessary to specify the heat release occurring during the detonation/combustion process. The usual practice has been to assume that the lower heating value of the fuel is a reasonable value to use. As mentioned in the Introduction, the real gas effects such as dissociation and recombination cause the sensible heat release to be

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less than the lower heating value of the fuel.<sup>1</sup> The decrease in heat release turns out to be a function of equivalence ratio, pressure and temperature as well as fuel type.

In this study, the sensible heat release during the detonation/combustion process was determined in two ways; the first being the value calculated from the CEA equilibrium code<sup>5</sup> and the second being the heat released based on finite rate reactions from the CFD code discussed in the next section. Unlike the equilibrium value, the finite rate heat release accounts for recombination and yields a higher heat release value.

The two values of the heat release were used in the cycle code to determine the specific thrust, fuel consumption and impulse for a hydrogen/air mixture at standard pressure and temperature. The equivalence ratios investigated were 0.6, 0.8, 1.0, and 1.15. The results consisted of two values of each of the performance parameters, one based on the equilibrium heat release and the other on the finite rate heat release.

The propulsion performance parameters were then interpreted under the premise that the equilibrium heat release did not reflect the influence of recombination on heat release and hence, yields a lower than maximum performance for the PDE. On the other hand, the finite rate heat release, which properly accounts for both dissociation and recombination, will yield the upper limit of performance potential for a PDE cycle.

#### CFD Analysis

The CFD analysis used was developed by Yungster and Radhakrishnan.<sup>6-8</sup> The code solves the axisymmetric Navier Stokes equations including finite rate chemistry and real gas effects using an implicit, total-variation diminishing (TVD) algorithm. The code includes a generalized detailed chemistry capability, various options for turbulence models, and steady state or time accurate marching algorithms. For this study, the viscous forces were not included and, therefore the Euler equations were actually used to perform single cycle calculations.

The numerical method used for solving the governing equations is described in detail in reference 6. Briefly, the equation set is discretized using a fully implicit, first order time accurate, variable-step backward differentiation formula method. The numerical fluxes are discretized using a second order spatially accurate TVD scheme. The resulting equations are then linearized in a conservative manner and solved iteratively, by using a lower-upper relaxation procedure

consisting of successive Gauss-Seidel (LU-SGS) sweeps.

The chemical reaction mechanism for hydrogen-air combustion was based on Jachimowski's model<sup>9</sup> and consists of 27 elementary reactions among 12 species. The inversion of large matrices is avoided by partitioning the system into reacting and non-reacting parts. Consequently, the matrices that have to be inverted are of the same size as those that arise in the commonly used point implicit methods. An important advantage of the present method is that it is stable for large CFL values, thereby enabling the use of large time steps to minimize computational cost.

In order to maintain good resolution of the detonation front at all times a multi-level, dynamically adaptive grid was used in which a very fine sub-grid continuously slides along with the detonation wave front.<sup>8</sup> This approach avoided the use of thousands of grid points.

The CFD finite rate calculations were used to compute the species evolution and the resulting thrust and impulse. They were also used to determine the sensible heat release occurring during the detonation and combustion processes for the hydrogen-air mixtures at the same equivalence ratios used in the thermo cycle analyses.

#### Comparative Analysis

The comparison of the cycle code and the CFD calculations was carried out as shown in figure 1. The cycle analysis used the sensible heat release determined from EQL to calculate the performance parameters and then used the finite rate value from the CFD to yield a second set of values. It is the second set, which is based on the finite rate heat release, that are believed to yield the maximum performance (upper cycle) limits for a PDE.

In the CFD analysis, detonation is initiated in a one meter length tube with a diameter of 6.6 centimeters using a 2 cm zone of high temperature nitrogen at 2500K and 40 bar. The tube is filled with hydrogen/air at 298K and 1 bar. This starting transient is neglected in the "ignition corrected" values of performance, whereas, in the "uncorrected results," the transient was included. This correction is justified on the basis of the need to introduce an ignition mechanism to obtain detonation, which creates an artificial force that is not representative of the actual ignition process<sup>3</sup>. The resulting values of the corrected parameters are believed to be representative of the flow geometry being analyzed. Figure 2 (from ref. 3) shows the result

of the ignition correction. Further efforts are underway to reduce the size of the ignition source and the corresponding correction required.

#### System Analyzed

For the thermodynamic cycle, it is assumed that the inlet has no losses and operates in an isentropic manner. The pressure and temperature are at standard conditions for this example. There is no ram pressure since the forward velocity is zero, i.e. static thrust conditions. The nozzle, which may be of any shape, is also assumed to be isentropic, yielding the maximum thrust for the operating conditions of the detonation chamber. Although a nozzle geometry having this characteristic is unknown at this time, it is not required for a cycle calculation, which seeks the upper performance capability of a PDE.

For the CFD analysis, the inlet again is assumed to have no losses. Admission of fuel and air occurs with no entropy generation. In fact, for the analysis, it is assumed that the detonation chamber is closed at the front end for the single cycle being analyzed.

However, in order to perform the CFD analysis a description of the geometry at the downstream end is required. In the absence of any specific design, it is assumed that the detonation chamber is open at the downstream end and has a constant diameter throughout and discharges to an ambient pressure of 1 bar. In this case, the CFD analysis, with the proper boundary conditions, should yield the “actual” performance for that geometry subject to the approximations in the solved equations, including the neglect of viscous effects. The term “actual” in this case refers to the fact that the expansion process is not isentropic. Hence, the difference between the thermo cycle analysis and the CFD will be due to the non-isentropic nozzle expansion losses and some frictional effects.

The analyzed geometry, therefore, is as shown in figure 3.

### Results

#### Sensible Heat Release

The heat releases calculated using the equilibrium code of Gordon and McBride,<sup>5</sup> and the finite rate CFD chemistry model are shown in figure 4. The differences in the two curves are due to the recombination that occurs as the heated gases burn and flow out of the detonation tube. As the gases recombine, additional heat is released.

The loss in sensible heat is found to be much larger at the higher equivalence ratios and is primarily due to the higher detonation temperatures reached. For an equivalence ratio of 0.6, the detonation temperature is 2422K and for a value of 1.15, the temperature reaches 2967K.

#### Thermo Cycle and CFD Analyses

Using the above variation of heat release values, the thermo cycle code yields the fuel specific impulse results shown in figure 5. As noted previously, the higher sensible heat associated with finite rate chemistry lead to higher values of impulse than those associated with equilibrium chemistry.

It is the performance associated with the finite rate results that are interpreted as the upper limit of PDE propulsion performance.

The ignition corrected results from the CFD analysis are shown in figure 6. As stated previously, the artificial force created by the ignition effect is not considered representative of the actual ignition process, and the resulting values of the ignition corrected values are believed to be accurate for the flow geometry being analyzed.

As stated in the Analyses section under Thermodynamic Cycle, the interpretation of the results is that the equilibrium heat release does not reflect the influence of recombination on heat release and hence, yields a lower than maximum performance for the PDE. On the other hand, use of the finite heat release in the thermo cycle, which correctly accounts for both dissociation and recombination, yields the upper cycle limit for the propulsion performance of a PDE cycle.

Plotting the thermo cycle finite rate result from figure 5 and the CFD ignition corrected finite rate results from figure 6 yields the plot shown in figure 7.

The differences in the two curves of figure 7 represent the losses principally incurred by the open-ended detonation tube and the nature of the non-isentropic expansion. The losses are on the order of 5 percent (250 seconds) of the impulse.

It is interesting to observe that the ratio of the impulse values from the CFD to the impulse value of the thermo cycle calculations, ( $I_{CFD}/I_{thermo}$ ), have values from 0.94 to 0.95. It is informative, therefore, to look at the values determined by the cycle analysis using a nozzle efficiency of 0.95. When these calculations are performed, the impulse values turn out to be 6 percent lower, which is close to our expectations.

The differences in the two curves of figure 7, which are taken to be the real performance versus the potential performance, are seen to amount to values between 200 and 300 seconds. These differences, once again, emphasize the critical nature of the nozzle exhaust design in order to achieve the potential gain in PDE propulsion performance.<sup>4</sup>

#### Comparison with Experimental Data

The data obtained in this study were compared to that obtained at the Wright Labs by Schafer, Stutrud and Bradley.<sup>10</sup> In figure 8, our data points (from figure 7 described above) are shown on a copy of the impulse versus equivalence plot from figure 12 of reference 10. The open squares represent our thermo cycle upper performance limit and the open diamond symbols represent our ignition corrected finite rate CFD results. The CFD results are in excellent agreement with the data and the cycle results show the potential improvement. *Note that the differences were more clearly depicted in figure 7.* Also shown in the figure are the results for a single cycle PDE engine (open-ended tube) based on a model using gas dynamic calculations and experimental results.<sup>11</sup>

#### Specific Thrust and Fuel Consumption

The specific thrust and fuel consumption were also determined using the cycle analysis and are shown in figures 9 and 10. In these calculations, only the finite rate heat release values were used. These results represent the maximum or upper limit values for the thrust and fuel consumption, as was the case for the impulse values.

#### Conclusions

A combination of a thermodynamic cycle and a CFD finite rate code were used to analyze detonation behavior in order to establish an upper limit for PDE cycle performance.

The thermo cycle code was used with both equilibrium and finite rate sensible heat release values. It was determined that the recombination occurring during the detonation/combustion process required the use of the finite rate values to accurately capture the real gas effects.

The CFD finite rate heat release was found to be high due to the ignition mechanism, which caused a large force that is not representative of the actual ignition process. These values were corrected and used for determining propulsion parameters, which in turn, were compared with the thermo cycle finite rate results. The comparisons established the cycle upper limits for PDE performance and the potential gains that may be realized in PDE nozzle design.

Comparison with available data showed agreement with both the cycle analysis, namely the maximum upper limit values, and between the CFD and experimental data, namely the actual performance.

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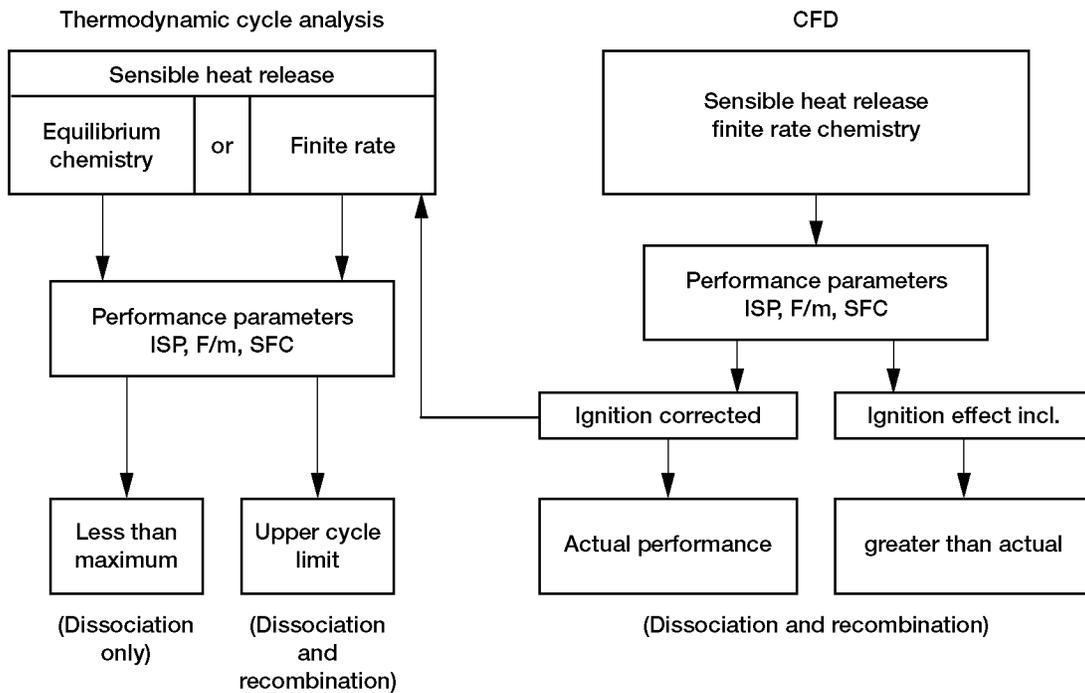


Figure 1.—Block diagram illustrating the comparative analyses.

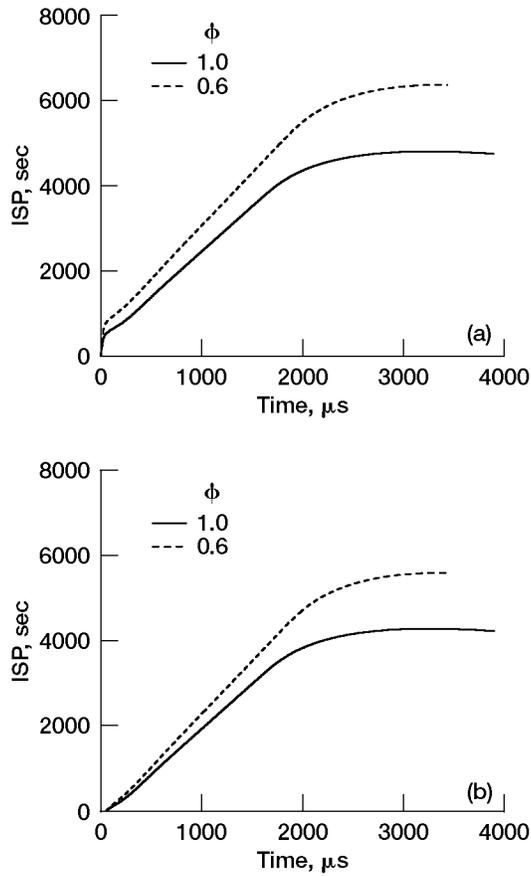


Figure 2.—Comparison of specific impulse between the finite rate chemistry computations for  $\phi = 1.0$  and  $\phi = 0.6$ . In part (b), the force produced during the starting transient phase (first 50  $\mu$  sec) was neglected.

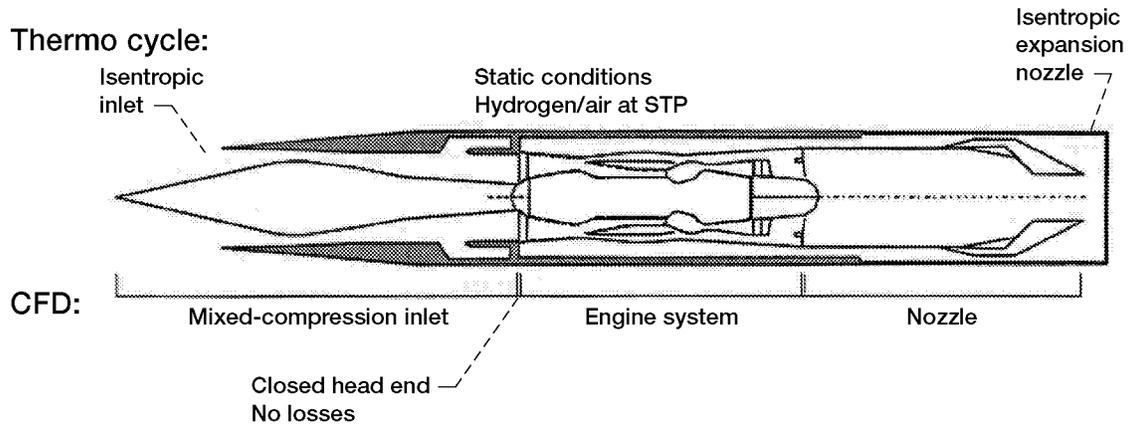


Figure 3.—Comparison of model geometries for notional engine.

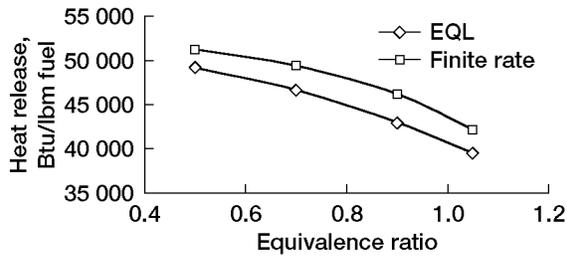


Figure 4.—Heat release determined from EQL and CFD analysis.

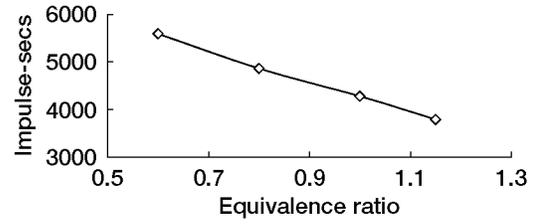


Figure 6.—Impulse calculated from CFD analysis.

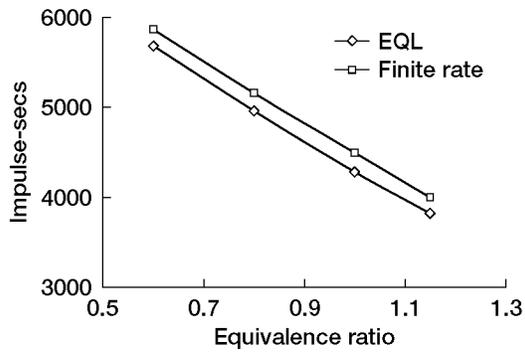


Figure 5.—Impulse calculated from cycle analysis.

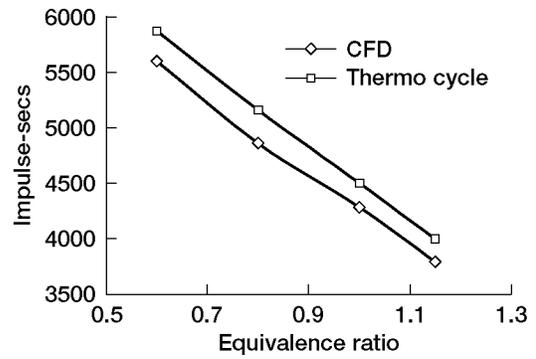


Figure 7.—Potential improvement in impulse-actual and upper limit values.

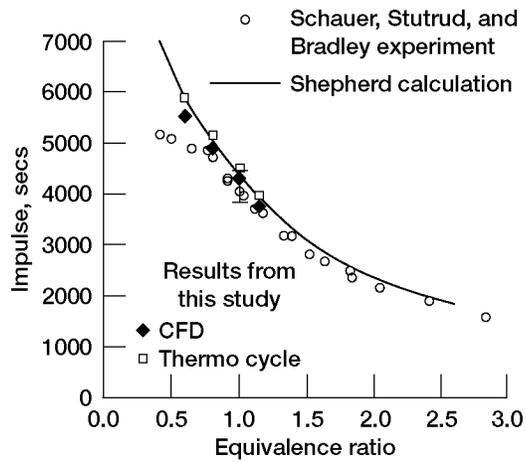


Figure 8.—Calculated cycle and CFD impulse superposed on figure 12 of reference 10.

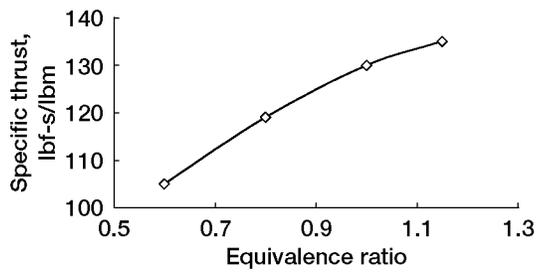


Figure 9.—Specific thrust from cycle analysis with finite rate heat release.

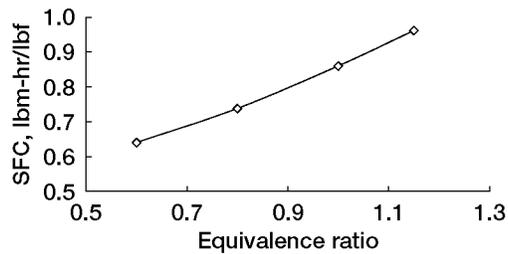


Figure 10.—Specific fuel consumption-cycle analysis with finite rate heat release.

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